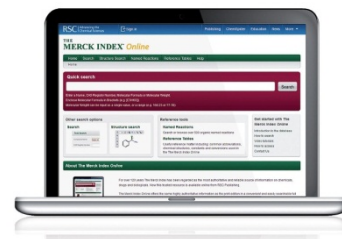


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Home

Quick search

Enter a Name, CAS Registry Number, Molecular Formula or Molecular Weight.
Enclose Molecular Formula in Brackets (e.g. [C₃H₆O]).
Molecular Weight can be input as a single value, or a range (e.g. 168.23 or 77-78)

Other search options

Search

Text Search

Compound Name

CAS Registry Number

Structure search

Reference tools

Named Reactions
Search or browse over 500 organic named reactions

Reference Tables
Useful reference matter including: common abbreviations, chemical structures, constants and conversions used in the The Merck Index* *Online*

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Quick search

- Quickly search The Merck Index *Online* using the box on the home page and at the bottom of individual records.

Quick search

Search

Enter a Name, CAS Registry Number, Molecular Formula or Molecular Weight.
Enclose Molecular Formula in Brackets (e.g. [C₃H₆O]).
Molecular Weight can be input as a single value, or a range (e.g. 168.23 or 77-78)

Advanced search

- Click **Search** to find records based on detailed properties, including uses, melting points and molecular weights
- Narrow your search by entering search terms in more than one field

THE MERCK INDEX[®] *Online*

Home **Search** Structure Search Named Reactions Reference Tables My Records Help

Home > Search

Search Guidelines

You may use "=" prefix in text fields to specify exact query matching (e.g. "=acetic acid")
You can enter parameters in multiple fields to refine your searches.
Quick help can be accessed by clicking on the ? symbol next to any field, or See [Help](#) for further details.

Text Search

Compound Name	<input type="text"/>	?	Non-Medical Uses	<input type="text"/>	?
CAS Registry Number	<input type="text"/>	?	Human Therapeutic Use	Select Category	?
Literature References and Notes	<input type="text"/>	?	Manufacturer	<input type="text"/>	?
Veterinary Therapeutic Use	<input type="text"/>	?	Full Text	<input type="text"/>	?

Properties Search

Molecular Formula	<input type="text"/>	?	Density (specific gravity)	<input type="text"/>	+/-	0.5	?				
Molecular Weight	<input type="text"/>	g/mol	+/-	0.5	?	Index of Refraction	<input type="text"/>	+/-	0.01	?	
Boiling Point	<input type="text"/>	°C	+/-	0.5	?	Optical Rotation	<input type="text"/>	+/-	0.2	?	
Melting Point	<input type="text"/>	°C	+/-	0.5	?	Flash Point	<input type="text"/>	°C	+/-	0.5	?
pKa	<input type="text"/>	+/-	0.25	?	Absorption Max	<input type="text"/>	nm	+/-	1	?	
Log P	<input type="text"/>	+/-	0.25	?	Toxicity	<input type="text"/>	mg/kg	+/-	10	?	

Search Clear

Structure search

- Use the **Options** on the right to search the exact structure, as a substructure, or for similar structures
- Reduce the number of results by combining substructure or similarity searches with an advanced **Text** or **Properties Search**

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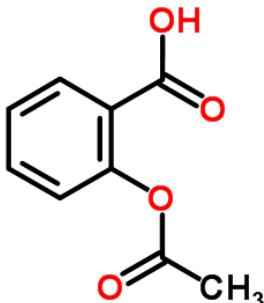
Home Search **Structure Search** Named Reactions Reference Tables My Records Help

Home > Structure Search

Search Guidelines

You can draw in a structure as the basis for an exact search or as the starting point for a substructure or similarity search. It is possible to combine substructure and similarity searches with some text and property searches. See [Help](#) for further details.

Convert Edit



Options

- Exact Search
- Substructure Search
 - ☒ Match specified tautomer
 - ☐ Match all tautomers
- Similarity Search

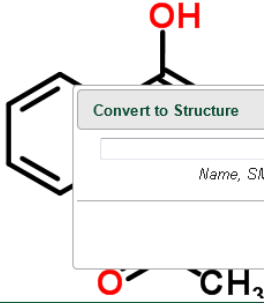
Search

Text Search

Compound Name Non-Medical Uses

- Click **Convert** to create a structure from a chemical name, or from a SMILES or InChI descriptor

Convert Edit



Options

- Exact Search
- Substructure Search
 - ☒ Match specified tautomer
 - ☐ Match all tautomers
- Similarity Search

Convert to Structure

Name, SMILES or InChI

Ok Cancel

- Click **Edit** draw your own structure or substructure

The screenshot displays the 'Edit Structure' window of the JChemPaint software. The window has a menu bar at the top with options: Home, Search, Structure Search, Named Reactions, Reference Tables, My Records, and Help. Below the menu bar is a toolbar with various drawing tools. Two red callout boxes highlight specific tools: one points to the 'Clear structure' button (represented by a trash can icon) and the other points to the 'Delete individual atoms or bonds' button (represented by a scissors icon). The main drawing area contains a chemical structure of 2-acetoxybenzoic acid, which consists of a benzene ring with a carboxylic acid group (-COOH) and an acetoxy group (-O-C(=O)-CH₃) attached at adjacent positions. On the left side of the window, there is a vertical list of chemical elements: H, C, N, O, S, P, F, Cl, Br, and a bullet point. At the bottom right of the window are 'Ok' and 'Cancel' buttons.

Search results

- The search results page shows records that match the search criteria, for example **2461 results** match the word 'benzene'
- Structures, molecular weights and molecular formulae are displayed if available
- Click the name of the compound to open the record

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[Home](#) | [Search](#) | [Structure Search](#) | [Named Reactions](#) | [Reference Tables](#) | [My Records](#) | [Help](#)

Home > Search result

Your search returned **2461 results**, based on the following search criteria:
Name: **benzene**

[Change this query](#) [Start a new search](#) [Save this query](#)

Your recent search

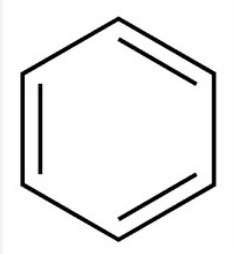
benzene
"acetic acid"
Compound Name:acetic
acetic acid
ethanol
Compound Name:acetic acid
Compound Name:aspirin

☐ Select All [Add to My Records](#) Results per page **20** Page **1** of 124 [Go](#)

☐ Benzene

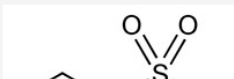
Molecular Weight: 78.11
Molecular Formula: C_6H_6

Open In : [New Window](#) [New Tab](#) [Add to My Records](#)



☐ Benzenesulfonyl Chloride

Molecular Weight: 176.61
Molecular Formula: $C_6H_5ClO_2S$



Monograph records

- Basic properties such as CAS Registry number, synonyms, trade names, molecular formula and molecular weight are listed at the top
- The chemical structure is listed on the right, which can be downloaded as jpg or mol files

Benzene
Print view
Add to My Records
Back to search results

Monograph ID: MONO1500001068
Title: Benzene
CAS Registry Number: 71-43-2
Additional Names: Benzol, cyclohexatriene
Molecular Formula: C₆H₆
Molecular Weight: 78.11
Percent Composition: C 92.26%, H 7.74%
Standard InChI: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
Standard InChIKey: UHOVQNZJYSORNB-UHFFFAOYSA-N

Save
Image Structure Zoom

Properties
 Clear, colorless, volatile liquid; characteristic odor. d_4^{15} 0.8787. bp 80.1°C. mp 5.5°C. n_D^{20} 1.50108. Flash pt, closed cup: 12°F (-11°C). Sol in water at 23.5°C (w/w): 0.188%. Flammable. Miscible with alc, chloroform, ether, carbon disulfide, carbon tetrachloride, glacial acetic acid, acetone, oils. Keep in well-closed containers in a cool place and away from fire. LD₅₀ orally in young adult rats: 3.8 ml/kg (Kimura).

- Authorised users can view additional data including chemical and physical **Properties and Uses**
- **References** to the published literature are given, e.g. for isolations, syntheses, clinical trials etc.
- **DOI** and **PubMed ID** numbers are included and link to the original article

Properties

Clear, colorless, volatile liquid; characteristic odor. d_4^{15} 0.8787. bp 80.1°C. mp 5.5°C. n_D^{20} 1.50108. Flash pt, closed cup: 12°F (-11°C). Sol in water at 23.5°C (w/w): 0.188%. Flammable. Miscible with alc, chloroform, ether, carbon disulfide, carbon tetrachloride, glacial acetic acid, acetone, oils. Keep in well-closed containers in a cool place and away from fire. LD₅₀ orally in young adult rats: 3.8 ml/kg (Kimura).

Use

Manuf of industrial chemicals such as polymers, detergents, pesticides pharmaceuticals, dyes, plastics, resins. Organic solvent for waxes, resins, oils, natural rubber, etc. Reference for quantitating compds. Gasoline additive.

References

Natural component of petroleum, usually <1.0% by weight. Discovered by Faraday in compressed oil gas in 1825. Obtained in the coking of coal and in the production of illuminating gas from coal. Manuf by catalytic reforming and separation of aromatic compounds, thermal or catalytic dealkylation of toluene, toluene disproportionation, from pyrolysis gasoline. Purification by washing with water: **GB 863711** (1961 to Schloven-Chemie and H. Koppers GmbH), *C.A.* **55**, 16971f (1961). Lab prepn from aniline: Gattermann-Wieland, *Praxis des Organischen Chemikers* (de Gruyter, Berlin, 40th ed., 1961) p 247. Production of pure benzene: French, *Ind. Chem.* **39**, 9-12 (1963). Manuf. *Faith, Keyes & Clark's Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 126-137. Physical properties: Thorne *et al.*, *Ind. Eng. Chem. Anal. Ed.* **17**, 481 (1945) DOI: 10.1021/i560144a006. Solubility studies: F. P. Schwarz, *Anal. Chem.* **52**, 10 (1980) DOI: 10.1021/ac50051a004. Toxicity data: Kimura *et al.*, *Toxicol. Appl. Pharmacol.* **19**, 699 (1974) DOI: 10.1016/0041-008X(71)90301-2 PMID: 5132037. Review: W. Fruscella in *Kirk-Othmer Encyclopedia of Chemical Technology*, 4th edn, Interscience, New York, 1990, pp 73-100. Review of

- Therapeutic categories and other keywords are given under **Classifications**
- Additional **Notes** such as safety information may be available
- Data for **Related Compounds** such as derivatives, salts or stereoisomers are given if they do not have their own record

0, 117-200 (1999), and human exposure. *Toxicological Profile for Benzene* (1999-2004, 2007) 430 pp. Symposium on metabolism, toxicity and carcinogenesis: *Environ. Health Perspect.* **82**, 3-310 (1989); *ibid.* **104**, Suppl. 6, 1121-1441 (1996).

Classifications

Therapeutic Category (Vet.): Has been used as a disinfectant.

Notes

Caution: Potential symptoms of overexposure by inhalation or ingestion are dizziness, headache, vomiting, visual disturbances, staggering gait, hilarity, fatigue, anorexia, lassitude, CNS depression, loss of consciousness, respiratory arrest. Chronic exposure has been associated with bone marrow depression and leukemia. Direct contact may cause irritation of eyes, nose, respiratory system and skin; dermatitis may develop due to defatting action. Aspiration into the lung may lead to chemical pneumonitis. See *Patty's Industrial Hygiene and Toxicology* vol. **2B**, G. D. Clayton, F. E. Clayton, Eds. (Wiley-Interscience, New York, 4th ed., 1994) pp 1306-1326; *NIOSH Pocket Guide to Chemical Hazards* (DHHS/NIOSH 97-140, 1997) p 26. Benzene is listed as a known human carcinogen: *Report on Carcinogens, Twelfth Edition* (PB2011-111646, 2011) p 60.

Related Compounds



Derivative Type: Sodium salt
CAS Registry Number: 1623-99-0
Additional Names: Phenyl sodium

Named reactions

- Over 500 **Named Reactions** are listed and can be searched by name or browsed by initial letter
- The record for each reaction includes a description, scheme and representative references

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Home Search Structure Search **Named Reactions** Reference Tables My Records Help

Home > Reaction > Reaction Results

Browse by First Letter

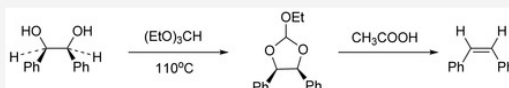
A B C D **E** F G H I J K L M N O P Q R S T U V W X Y Z 0..9 # \$ % ^ & @

Browsing reactions beginning with E

Results per page 20

Page 1 of 1 Go

Eastwood Reaction



Open In : New Window New Tab

Edman Degradation



Reference tables

- Useful supplementary information defining common chemical terms and conventions are available in pdf format in the **Reference Tables**

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Home	Search	Structure Search	Named Reactions	Reference Tables	My Records	Help
Home > Reference Tables						

The links below provide access to useful information relating to general chemistry database. They are based upon the appendices provided in the print edition.

- Acronyms
- Alchemical Symbols Used in Biology and Botany
- Amino Acids Found in Proteins
- Atomic Weights Order of Atomic Number
- Chemical Terms Translator
- Common Heterocyclic Ring Systems
- Fundamental Physical and Mathematical Constants
- Glossary
- **Greek Alphabet**
- International Patent Country Codes
- International System of Units (SI)
- Latin Terms

Greek Alphabet							
Name of Letter	Capital	Lower Case	Transliteration	Name of Letter	Capital	Lower Case	Transliteration
alpha	A	α	a	nu	Ν	ν	n
beta	B	β	b	xi	Ξ	ξ	x
gamma	Γ	γ	g	omicron	Ο	ο	o short
delta	Δ	δ	d	pi	Π	π	p
epsilon	Η	ε	e short	rho	Ρ	ρ	r
zeta	Ζ	ζ	z	sigma	Σ	σ or ς	s
eta	Η	η	e long	tau	Τ	τ	t
theta	Θ	θ	th	upsilon	Υ	υ	y
iota	Ι	ι	i	phi	Φ	φ or ϕ	f
kappa	Κ	κ	k, c	chi	Χ	χ	ch as in German echt
lambda	Λ	λ	l	psi	Ψ	ψ	ps
mu	Μ	μ	m	omega	Ω	ω	o long

- Russian Alphabet
- Selected Hexoses and Pentoses
- Table of Minerals
- Terms for Radicals and Groups Used for Nonproprietary Names
- Thermometric Equivalents
- Universal Conversion Factors
- Vaccines

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My Records

- If you are logged in, you can save your favourite searches and monographs by clicking the **Add to My Records** button
- You can save to the default list, previously created custom lists or a new list

Benzene Print view Add to My Records Back to search results

Monograph ID: MONO1500001068
Title: Benzene
CAS Registry Number: 71-43-2
Additional Names: Benzol, cyclohexatriene
Molecular Formula: C₆H₆

My Default List
Analgesics
Photosensitizers
Add a new list

- Click **My Records** to view your saved searches and monographs

Home Search Structure Search Named Reactions Reference Tables **My Records** Help

Home > My Records

My Records

Items Per Page: 10 Page 1 of 1 Go

My Saved Queries

Search Contents	Created On	Delete
Molecular Formula:C6H12O6	30/09/2013 13:41:45	

Recent Searches

Search Contents	Created On
Compound Name:benzene	26/11/2013 18:50:27
Compound Name:acetic acid	26/11/2013 17:56:18

- Pay-per-view monographs are automatically saved in the **Purchased Monographs** section
- You can share links to a saved list of records by **Email**

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You have not purchased any monographs

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Glucose	
Starch	

Analgesics Email Edit Delete Items Per Page: 10 Page 1 of 1 Go

Acetaminophen	
Aspirin	